Elasticity of superhydrous phase B at high temperature and pressure: Implications for water flow into lower mantle

Dapeng Yang, Wenzhong Wang, Zhongqing Wu*

Laboratory of Seismology and Physics of Earth's Interior, School of Earth and Space Sciences, University of Science and Technology of China, Hefei 230026, China * wuzq10@ustc.edu.cn

Superhydrous phase B (ShyB) (Mg₁₀Si₃O₁₄(OH)₄), as one of the dense hydrous magnesium silicate phases, is considered to be an important candidate for transporting water into the transition zone and lower mantle since it is stable up to ~ 31 GPa and 1400 $^{\circ}$ C. The thermodynamic and elastic properties of ShyB at relevant mantle conditions were obtained by firstprinciple calculation based on density function theory. The calculated results such as the equation of states and elasticity are in good agreements with available experimental results. Zero motion and room temperature increase the equilibrium volume by 1.4% and reduce the V_P and V_S by 1.3% and 1.4%, respectively. The temperature sensitivity of sound velocities decreases with increasing pressure. ShyB has far lower velocity and density than iron-free bridgmanite (MgSiO₃) and periclase, which implies that the accumulation of shyB will generate the lowvelocity anomaly in the uppermost lower mantle. With these elastic data, we discussed in detail the seismic feature of ShyB and seismic evidence of ShyB in the uppermost lower mantle